Full wwPDB X-ray Structure Validation Report ⓘ

Dec 28, 2022 – 02:03 PM EST

PDB ID	:	7K75
Title	:	Crystal structure of MAD2-6 IgA Fab in complex with PfCSP N-terminal peptide.
Authors	:	Pholcharee, T.; Wilson, I.A.
Deposited on	:	2020-09-22
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

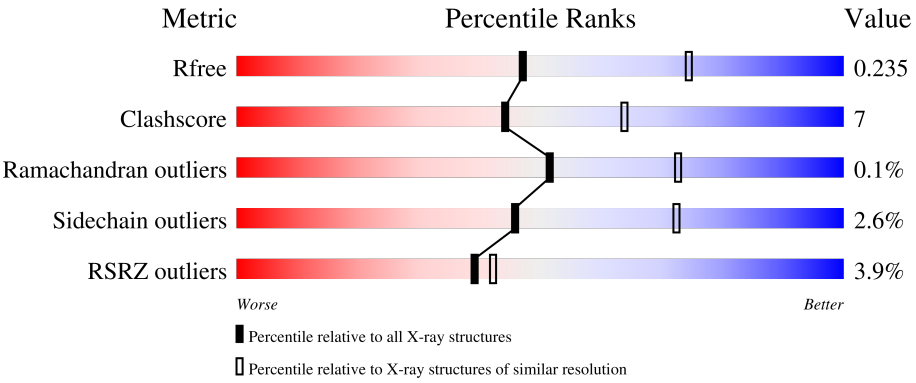
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	225	% 80% 20%
1	C	225	% 82% 18%
1	I	225	12% 74% 24% ••
1	M	225	11% 80% 18% •
2	B	213	84% 16%

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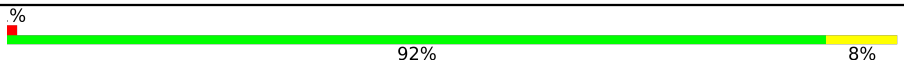
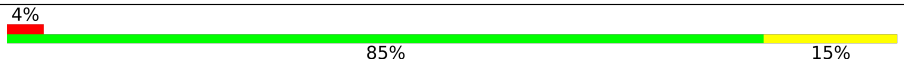
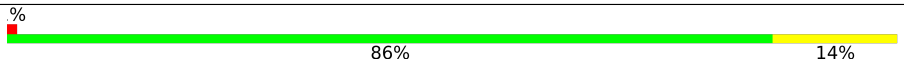
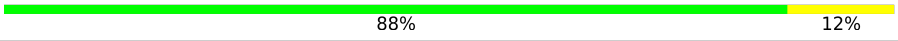
Mol	Chain	Length	Quality of chain
2	D	213	
2	J	213	
2	N	213	
3	E	8	
3	F	8	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13557 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Heavy chain of MAD2-6 IgA Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	2	0
			1701	1078	282	333	8			
1	C	225	Total	C	N	O	S	0	0	0
			1683	1069	277	329	8			
1	I	222	Total	C	N	O	S	0	0	0
			1578	1007	260	303	8			
1	M	222	Total	C	N	O	S	0	1	0
			1647	1048	274	317	8			

- Molecule 2 is a protein called Light chain of MAD2-6 IgA Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1619	1009	274	329	7			
2	D	213	Total	C	N	O	S	0	1	0
			1621	1011	274	329	7			
2	J	213	Total	C	N	O	S	0	1	0
			1615	1006	272	330	7			
2	N	213	Total	C	N	O	S	0	1	0
			1612	1003	271	331	7			

- Molecule 3 is a protein called PfCSP N-terminal peptide P17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	0	0	0
			66	44	14	8			
3	F	8	Total	C	N	O	0	0	0
			66	44	14	8			

- Molecule 4 is water.

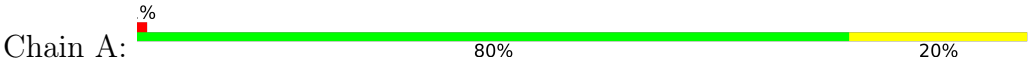
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	73	Total O 73 73	0	0
4	B	50	Total O 50 50	0	0
4	D	46	Total O 46 46	0	0
4	C	76	Total O 76 76	0	0
4	I	6	Total O 6 6	0	0
4	J	43	Total O 43 43	0	0
4	M	26	Total O 26 26	0	0
4	N	25	Total O 25 25	0	0
4	E	3	Total O 3 3	0	0
4	F	1	Total O 1 1	0	0

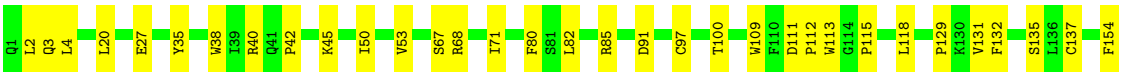
3 Residue-property plots (i)

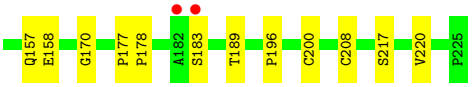
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Heavy chain of MAD2-6 IgA Fab

Chain A:

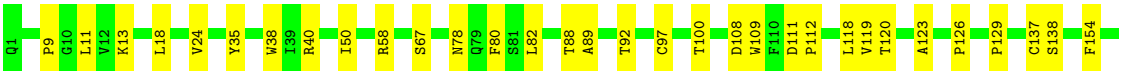


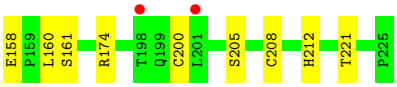




• Molecule 1: Heavy chain of MAD2-6 IgA Fab

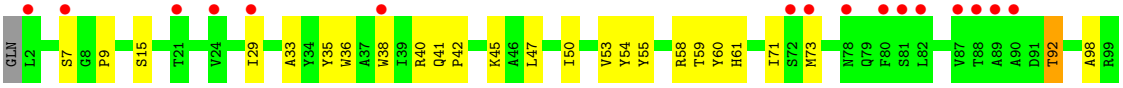
Chain C:

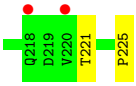




• Molecule 1: Heavy chain of MAD2-6 IgA Fab

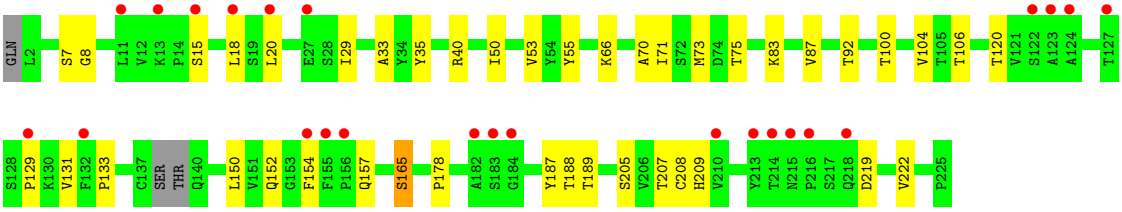
Chain I:



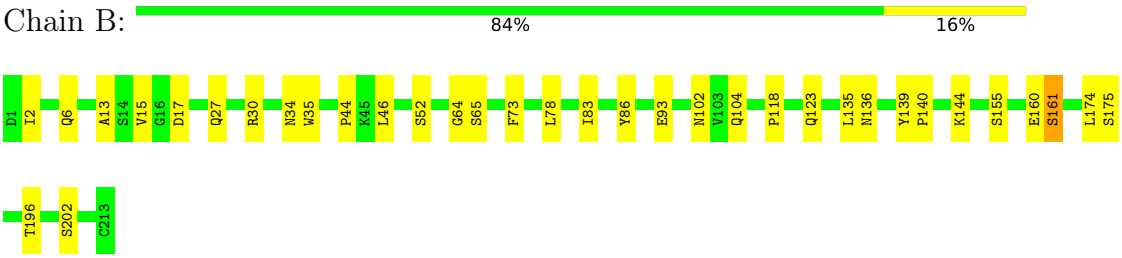


• Molecule 1: Heavy chain of MAD2-6 IgA Fab

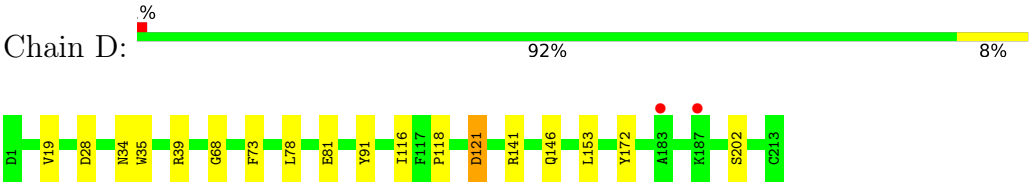
Chain M:



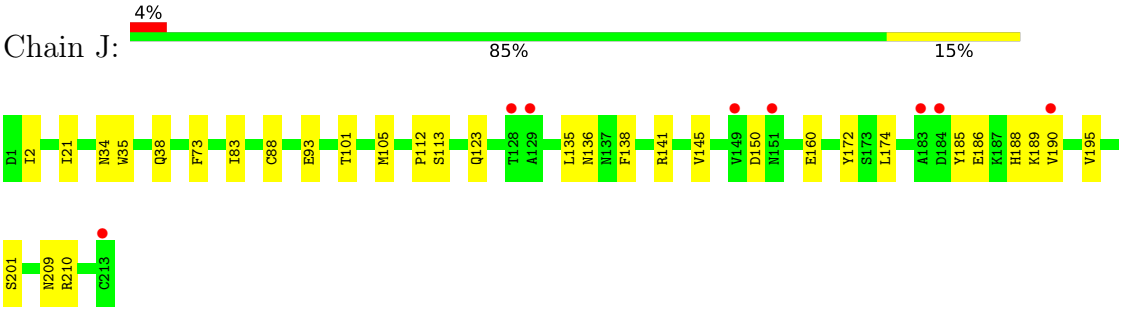
• Molecule 2: Light chain of MAD2-6 IgA Fab



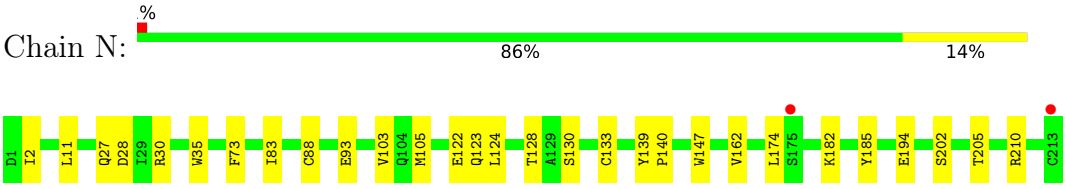
• Molecule 2: Light chain of MAD2-6 IgA Fab



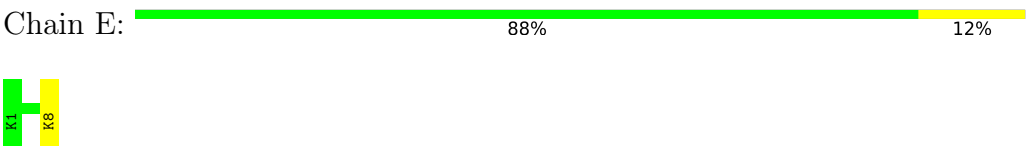
• Molecule 2: Light chain of MAD2-6 IgA Fab



• Molecule 2: Light chain of MAD2-6 IgA Fab



• Molecule 3: PfCSP N-terminal peptide P17



• Molecule 3: PfCSP N-terminal peptide P17

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.14Å 153.68Å 193.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.96 – 2.50 48.32 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.96-2.50) 98.9 (48.32-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.192 , 0.236 0.192 , 0.235	Depositor DCC
R_{free} test set	3739 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13557	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/1750	0.50	0/2408
1	C	0.26	0/1732	0.52	0/2384
1	I	0.27	0/1625	0.51	0/2249
1	M	0.26	0/1695	0.50	0/2334
2	B	0.27	0/1653	0.50	0/2248
2	D	0.27	0/1655	0.50	0/2251
2	J	0.28	0/1649	0.51	0/2246
2	N	0.27	0/1646	0.52	0/2243
3	E	0.22	0/67	0.42	0/86
3	F	0.24	0/67	0.37	0/86
All	All	0.27	0/13539	0.51	0/18535

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1701	0	1634	27	0
1	C	1683	0	1621	24	0
1	I	1578	0	1429	35	0
1	M	1647	0	1569	22	0
2	B	1619	0	1538	24	0
2	D	1621	0	1535	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1615	0	1512	29	0
2	N	1612	0	1505	16	0
3	E	66	0	81	1	0
3	F	66	0	81	1	0
4	A	73	0	0	2	0
4	B	50	0	0	0	0
4	C	76	0	0	0	0
4	D	46	0	0	0	0
4	E	3	0	0	0	0
4	F	1	0	0	0	0
4	I	6	0	0	0	0
4	J	43	0	0	0	0
4	M	26	0	0	0	0
4	N	25	0	0	0	0
All	All	13557	0	12505	170	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ILE:HD12	2:B:93:GLU:HB2	1.54	0.90
2:J:189:LYS:HE3	2:J:209:ASN:HB3	1.56	0.88
2:J:186:GLU:HA	2:J:210:ARG:HH11	1.42	0.83
2:B:15:VAL:HG11	1:C:9:PRO:HB3	1.60	0.82
1:M:92:THR:HG23	1:M:120:THR:HA	1.66	0.76
2:J:186:GLU:HA	2:J:210:ARG:NH1	2.01	0.75
1:C:13:LYS:HG2	1:C:123:ALA:HA	1.71	0.71
2:N:124:LEU:O	2:N:182:LYS:HD2	1.93	0.68
1:I:40:ARG:HB3	1:I:50:ILE:HD11	1.77	0.66
1:C:174:ARG:HH11	1:C:174:ARG:HG3	1.62	0.65
1:A:67:SER:O	1:A:85:ARG:NH1	2.30	0.65
1:A:131:VAL:HB	1:A:220:VAL:HG21	1.78	0.64
2:B:102:ASN:HD22	2:B:104:GLN:HE21	1.46	0.63
2:J:186:GLU:CA	2:J:210:ARG:NH1	2.62	0.62
1:M:8:GLY:HA3	1:M:20:LEU:HD23	1.82	0.61
2:J:160:GLU:HG2	2:J:174:LEU:HD21	1.83	0.61
1:M:152:GLN:HA	1:M:188:THR:HG23	1.83	0.60
1:A:42:PRO:HB2	1:A:45:LYS:HG3	1.85	0.58
1:I:129:PRO:HB3	1:I:154:PHE:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:213:TYR:HD2	1:I:214:THR:H	1.49	0.58
2:N:83:ILE:HD11	2:N:105:MET:HB2	1.85	0.58
1:A:177:PRO:O	2:B:161:SER:OG	2.22	0.57
2:J:83:ILE:HD11	2:J:105:MET:HB2	1.85	0.57
2:N:11:LEU:HD11	2:N:103:VAL:HG22	1.85	0.57
2:D:35:TRP:CE2	2:D:73:PHE:HB2	2.40	0.57
1:M:129:PRO:HB3	1:M:154:PHE:HB3	1.87	0.56
1:I:92:THR:HB	1:I:121:VAL:HG12	1.87	0.56
1:A:35:TYR:HB2	1:A:100:THR:HG23	1.88	0.56
1:M:33:ALA:O	3:E:8:LYS:NZ	2.32	0.56
2:N:194:GLU:HG3	2:N:205:THR:HG22	1.87	0.56
1:M:157:GLN:HB3	1:M:187:TYR:CD2	2.40	0.56
1:M:53:VAL:HB	1:M:71:ILE:HG12	1.89	0.55
2:N:2:ILE:HG12	2:N:27:GLN:HB2	1.88	0.54
1:A:40:ARG:HB3	1:A:50:ILE:HD11	1.89	0.54
2:D:39:ARG:NH1	2:D:81:GLU:O	2.33	0.54
1:I:134:LEU:HB2	1:I:148:ALA:HB3	1.89	0.54
1:I:134:LEU:HD11	1:I:150:LEU:HB2	1.88	0.54
1:A:20:LEU:HD12	1:A:82:LEU:HD23	1.89	0.54
2:B:35:TRP:CE2	2:B:73:PHE:HB2	2.42	0.54
1:M:104:VAL:HG12	1:M:106:THR:H	1.72	0.54
2:J:2:ILE:HD12	2:J:93:GLU:HB2	1.89	0.54
1:I:35:TYR:HB2	1:I:100:THR:HG23	1.89	0.54
2:J:186:GLU:O	2:J:210:ARG:NH1	2.40	0.54
1:A:68:ARG:NH2	1:A:91:ASP:OD2	2.39	0.53
1:C:174:ARG:HG3	1:C:174:ARG:NH1	2.24	0.53
1:I:132:PHE:CE1	2:J:123:GLN:HG3	2.44	0.53
1:C:35:TYR:HB2	1:C:100:THR:HG23	1.91	0.53
2:B:160:GLU:HG2	2:B:174:LEU:HD21	1.90	0.53
1:M:35:TYR:HB2	1:M:100:THR:HG23	1.91	0.52
1:C:11:LEU:HD12	1:C:126:PRO:HG3	1.90	0.52
2:D:146:GLN:CD	2:D:153:LEU:HD23	2.29	0.52
1:I:98:ALA:HB1	1:I:110:PHE:HB3	1.92	0.52
2:N:35:TRP:CE2	2:N:73:PHE:HB2	2.45	0.51
1:I:53:VAL:HB	1:I:71:ILE:HG12	1.93	0.51
2:N:185:TYR:CZ	2:N:210:ARG:HG3	2.44	0.51
1:A:137:CYS:HB2	2:B:118:PRO:HD3	1.92	0.51
2:J:186:GLU:CA	2:J:210:ARG:HH11	2.16	0.51
2:J:150:ASP:OD2	2:J:188:HIS:HB3	2.12	0.50
2:D:28:ASP:OD1	2:D:68:GLY:HA2	2.11	0.50
2:B:144:LYS:HB3	2:B:196:THR:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:136:LEU:HD23	1:I:140:GLN:HG3	1.93	0.50
2:J:35:TRP:CZ3	2:J:88:CYS:HB3	2.46	0.50
1:C:40:ARG:HB3	1:C:50:ILE:HD11	1.94	0.50
1:I:164:TRP:CG	1:I:193:LEU:HD13	2.47	0.50
1:A:157:GLN:NE2	4:A:304:HOH:O	2.44	0.50
2:B:135:LEU:C	2:B:136:ASN:HD22	2.15	0.50
1:I:58:ARG:HH11	1:I:58:ARG:HG2	1.77	0.49
1:M:40:ARG:HB3	1:M:50:ILE:HD11	1.94	0.49
1:M:178:PRO:HA	1:M:189:THR:HB	1.94	0.49
2:D:118:PRO:HD3	1:C:137:CYS:HB2	1.94	0.49
2:J:145:VAL:HG22	2:J:195:VAL:HG22	1.93	0.48
1:A:3:GLN:NE2	4:A:305:HOH:O	2.46	0.48
1:A:118:LEU:HD22	1:A:158:GLU:HB2	1.96	0.48
1:I:213:TYR:HD2	1:I:214:THR:HG23	1.78	0.48
2:J:141:ARG:HG3	2:J:172:TYR:CG	2.48	0.48
2:N:123:GLN:HE22	2:N:130:SER:HB2	1.79	0.48
2:J:35:TRP:CE2	2:J:73:PHE:HB2	2.48	0.48
1:C:80:PHE:CZ	1:C:97:CYS:HB2	2.49	0.47
1:M:18:LEU:HB2	1:M:87:VAL:HG11	1.96	0.47
1:I:109:TRP:HB3	2:J:34:ASN:ND2	2.30	0.47
1:A:53:VAL:HB	1:A:71:ILE:HG12	1.96	0.47
2:B:6:GLN:NE2	2:B:86:TYR:O	2.46	0.47
2:D:116:ILE:HG22	1:C:138:SER:HB3	1.96	0.47
1:A:178:PRO:HA	1:A:189:THR:HB	1.95	0.47
1:I:54:TYR:HB3	1:I:58:ARG:HB3	1.95	0.47
1:I:162:VAL:HG22	1:I:210:VAL:HG22	1.97	0.47
2:J:2:ILE:HD12	2:J:93:GLU:CB	2.44	0.47
1:A:68:ARG:HH22	1:A:91:ASP:CG	2.18	0.47
2:J:113:SER:HB2	2:J:136:ASN:HB2	1.96	0.47
1:I:29:ILE:HG22	1:I:36:TRP:CE2	2.49	0.47
2:J:35:TRP:CD2	2:J:73:PHE:HB2	2.49	0.47
2:D:91:TYR:CG	1:C:108:ASP:HA	2.49	0.46
1:A:113:TRP:CH2	2:B:44:PRO:HG2	2.51	0.46
2:B:139:TYR:CG	2:B:140:PRO:HA	2.51	0.46
1:M:209:HIS:HD2	1:M:219:ASP:OD1	1.99	0.46
1:C:118:LEU:HD22	1:C:158:GLU:HB2	1.98	0.46
1:I:58:ARG:HG2	1:I:58:ARG:NH1	2.30	0.46
1:A:129:PRO:HB3	1:A:154:PHE:HB3	1.97	0.45
2:D:121:ASP:N	2:D:121:ASP:OD1	2.48	0.45
2:J:186:GLU:HG2	2:J:210:ARG:HH11	1.81	0.45
2:N:122:GLU:OE2	2:N:122:GLU:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:TRP:CD1	2:B:46:LEU:HD22	2.52	0.45
2:D:141:ARG:HG3	2:D:172:TYR:CD1	2.52	0.45
1:I:140:GLN:HE22	1:I:225:PRO:HG2	1.80	0.45
1:C:92:THR:HG23	1:C:120:THR:HA	1.99	0.45
1:C:205:SER:HB3	1:C:221:THR:HG23	1.99	0.45
1:I:53:VAL:HG23	1:I:59:THR:HG22	1.98	0.45
1:I:213:TYR:CD2	1:I:214:THR:HG23	2.52	0.45
1:C:24:VAL:O	1:C:78:ASN:ND2	2.39	0.45
1:C:35:TYR:OH	1:C:58:ARG:NH2	2.50	0.45
2:N:162:VAL:HG22	2:N:174:LEU:HD12	1.98	0.45
1:M:165:SER:HB3	1:M:207:THR:H	1.81	0.44
1:I:41:GLN:OE1	2:J:38:GLN:NE2	2.44	0.44
1:I:41:GLN:HB2	1:I:47:LEU:HD23	1.99	0.44
1:I:193:LEU:HD23	1:I:195:LEU:HD21	1.98	0.44
1:I:58:ARG:NH1	1:I:60:TYR:OH	2.50	0.44
2:B:13:ALA:HB3	2:B:78:LEU:HD22	1.99	0.44
2:N:2:ILE:HD12	2:N:93:GLU:HB3	1.99	0.44
1:M:29:ILE:HD12	1:M:73:MET:HG3	2.00	0.43
2:J:210:ARG:HE	2:J:210:ARG:HB3	1.53	0.43
1:A:170:GLY:O	1:A:196:PRO:HD3	2.19	0.43
2:B:139:TYR:CD1	2:B:140:PRO:HA	2.54	0.43
2:J:135:LEU:HB2	2:J:174:LEU:HB3	2.00	0.43
1:I:205:SER:OG	1:I:221:THR:OG1	2.36	0.43
1:A:109:TRP:HB3	2:B:34:ASN:ND2	2.34	0.43
2:J:141:ARG:HG3	2:J:172:TYR:CD1	2.54	0.43
1:C:88:THR:OG1	1:C:89:ALA:N	2.52	0.43
1:C:38:TRP:CD1	1:C:82:LEU:HB2	2.54	0.43
1:A:80:PHE:CZ	1:A:97:CYS:HB2	2.54	0.42
2:J:190:VAL:HG22	2:J:209:ASN:OD1	2.19	0.42
2:B:83:ILE:O	2:B:83:ILE:HG13	2.18	0.42
1:I:108:ASP:OD1	1:I:109:TRP:N	2.47	0.42
1:M:209:HIS:CD2	1:M:219:ASP:OD1	2.71	0.42
2:D:34:ASN:ND2	1:C:109:TRP:HB3	2.34	0.42
2:B:17:ASP:HA	1:C:126:PRO:HD2	2.01	0.42
1:A:132:PHE:CE2	2:B:123:GLN:HG3	2.55	0.42
1:C:18:LEU:HD12	1:C:119:VAL:HG11	2.01	0.42
1:C:129:PRO:HB3	1:C:154:PHE:HB3	2.02	0.42
1:I:160:LEU:HD23	1:I:161:SER:N	2.34	0.42
2:J:112:PRO:HB3	2:J:138:PHE:HB3	2.02	0.42
1:M:55:TYR:HA	1:M:73:MET:SD	2.60	0.42
1:A:113:TRP:CZ2	2:B:44:PRO:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:TRP:CD2	2:B:73:PHE:HB2	2.56	0.41
1:M:70:ALA:HB3	1:M:83:LYS:HB2	2.02	0.41
1:A:2:LEU:HD13	1:A:27:GLU:HB3	2.01	0.41
2:N:139:TYR:CG	2:N:140:PRO:HA	2.55	0.41
2:J:185:TYR:CZ	2:J:210:ARG:HG3	2.55	0.41
2:J:186:GLU:C	2:J:210:ARG:NH1	2.74	0.41
1:M:157:GLN:HB3	1:M:187:TYR:CE2	2.55	0.41
1:A:38:TRP:CD1	1:A:82:LEU:HB2	2.56	0.41
1:A:4:LEU:O	1:A:115:PRO:HD3	2.21	0.41
1:A:111:ASP:HA	1:A:112:PRO:HA	1.84	0.41
2:B:64:GLY:O	1:M:66:LYS:NZ	2.54	0.41
1:I:55:TYR:HA	1:I:73:MET:SD	2.60	0.41
1:M:133:PRO:HB3	1:M:222:VAL:HG22	2.02	0.41
2:N:35:TRP:CZ3	2:N:88:CYS:HB3	2.56	0.41
1:I:42:PRO:HB2	1:I:45:LYS:HG3	2.02	0.41
1:I:156:PRO:HD2	1:I:213:TYR:HD1	1.86	0.41
2:B:30:ARG:NH2	2:N:28:ASP:HB3	2.36	0.40
2:B:135:LEU:HB2	2:B:174:LEU:HB3	2.02	0.40
1:C:160:LEU:HD12	1:C:212:HIS:HB2	2.03	0.40
2:N:35:TRP:CD2	2:N:73:PHE:HB2	2.56	0.40
2:N:133:CYS:HB2	2:N:147:TRP:CH2	2.56	0.40
1:C:111:ASP:HA	1:C:112:PRO:HA	1.89	0.40
1:I:29:ILE:HD12	1:I:73:MET:HG3	2.03	0.40
1:I:33:ALA:O	3:F:8:LYS:NZ	2.50	0.40
2:J:21:ILE:HD13	2:J:101:THR:HB	2.03	0.40
1:I:38:TRP:HD1	1:I:71:ILE:HD12	1.86	0.40
2:D:19:VAL:HG21	2:D:78:LEU:HD22	2.03	0.40
1:M:131:VAL:HA	1:M:150:LEU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/225 (100%)	215 (96%)	10 (4%)	0	100	100
1	C	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
1	I	218/225 (97%)	201 (92%)	16 (7%)	1 (0%)	29	48
1	M	219/225 (97%)	209 (95%)	10 (5%)	0	100	100
2	B	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
2	D	212/213 (100%)	205 (97%)	7 (3%)	0	100	100
2	J	212/213 (100%)	205 (97%)	7 (3%)	0	100	100
2	N	212/213 (100%)	201 (95%)	11 (5%)	0	100	100
3	E	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
All	All	1744/1768 (99%)	1664 (95%)	79 (4%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	9	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/194 (98%)	186 (97%)	5 (3%)	46	72
1	C	189/194 (97%)	185 (98%)	4 (2%)	53	78
1	I	160/194 (82%)	150 (94%)	10 (6%)	18	34
1	M	181/194 (93%)	175 (97%)	6 (3%)	38	64
2	B	181/187 (97%)	174 (96%)	7 (4%)	32	57
2	D	180/187 (96%)	178 (99%)	2 (1%)	73	89
2	J	178/187 (95%)	177 (99%)	1 (1%)	86	95
2	N	178/187 (95%)	175 (98%)	3 (2%)	60	82
3	E	7/8 (88%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	7/8 (88%)	7 (100%)	0	100 100
All	All	1452/1540 (94%)	1414 (97%)	38 (3%)	46 72

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	SER
1	A	183	SER
1	A	200	CYS
1	A	208	CYS
1	A	217	SER
2	B	27	GLN
2	B	52	SER
2	B	65	SER
2	B	155	SER
2	B	161	SER
2	B	175	SER
2	B	202	SER
2	D	121	ASP
2	D	202	SER
1	C	67	SER
1	C	161	SER
1	C	200	CYS
1	C	208	CYS
1	I	7	SER
1	I	15	SER
1	I	61	HIS
1	I	92	THR
1	I	120	THR
1	I	125	SER
1	I	128	SER
1	I	169	GLN
1	I	200	CYS
1	I	213	TYR
2	J	201	SER
1	M	7	SER
1	M	15	SER
1	M	75	THR
1	M	165	SER
1	M	205	SER
1	M	208	CYS
2	N	30	ARG

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Mol	Chain	Res	Type
2	N	128	THR
2	N	202	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	104	GLN
2	D	102	ASN
2	D	104	GLN
1	C	144	ASN
2	J	104	GLN
2	J	146	GLN
1	M	199	GLN
1	M	218	GLN
2	N	102	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	225/225 (100%)	0.04	2 (0%) 84 86	27, 40, 61, 92	0
1	C	225/225 (100%)	0.04	2 (0%) 84 86	26, 38, 67, 88	0
1	I	222/225 (98%)	0.92	28 (12%) 3 3	40, 78, 102, 123	0
1	M	222/225 (98%)	0.68	24 (10%) 5 5	38, 63, 84, 106	0
2	B	213/213 (100%)	0.10	0 100 100	27, 38, 56, 68	0
2	D	213/213 (100%)	0.19	2 (0%) 84 86	25, 39, 62, 74	0
2	J	213/213 (100%)	0.27	8 (3%) 40 43	29, 44, 82, 90	0
2	N	213/213 (100%)	0.18	2 (0%) 84 86	34, 52, 79, 101	0
3	E	8/8 (100%)	0.02	0 100 100	38, 44, 53, 67	0
3	F	8/8 (100%)	-0.28	0 100 100	36, 39, 51, 60	0
All	All	1762/1768 (99%)	0.30	68 (3%) 39 42	25, 46, 86, 123	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	213	TYR	4.4
1	I	184	GLY	4.4
2	J	129	ALA	4.3
1	M	213	TYR	4.1
1	I	214	THR	3.9
1	I	7	SER	3.8
1	I	88	THR	3.8
1	I	186	LEU	3.7
1	I	90	ALA	3.7
1	M	216	PRO	3.5
1	I	89	ALA	3.5
1	M	11	LEU	3.5
2	N	213	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	121	VAL	3.4
1	M	18	LEU	3.3
1	M	155	PHE	3.3
1	I	73	MET	3.2
1	I	80	PHE	3.1
1	I	220	VAL	3.1
1	I	87	VAL	3.1
1	I	2	LEU	3.0
1	I	137	CYS	3.0
1	I	183	SER	3.0
1	A	183	SER	2.9
1	M	154	PHE	2.9
1	I	29	ILE	2.8
2	J	183	ALA	2.8
1	M	215	ASN	2.8
1	I	129	PRO	2.8
1	M	122	SER	2.8
1	C	198	THR	2.7
1	M	124	ALA	2.7
1	M	214	THR	2.7
1	M	123	ALA	2.6
2	J	128	THR	2.6
2	N	175[A]	SER	2.6
1	I	81	SER	2.6
2	J	213	CYS	2.6
1	M	218	GLN	2.5
1	M	127	THR	2.4
2	D	183	ALA	2.4
1	M	132	PHE	2.4
1	I	218	GLN	2.4
1	I	182	ALA	2.3
1	M	27	GLU	2.3
2	J	151	ASN	2.3
1	I	72	SER	2.3
1	I	24	VAL	2.3
1	I	78	ASN	2.2
1	C	201	LEU	2.2
1	M	129	PRO	2.2
1	M	13	LYS	2.2
1	I	38	TRP	2.2
1	M	210	VAL	2.2
1	M	20	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	15	SER	2.1
1	I	206	VAL	2.1
1	M	184	GLY	2.1
1	I	82	LEU	2.1
1	M	182	ALA	2.1
2	D	187	LYS	2.1
1	A	182	ALA	2.0
1	I	21	THR	2.0
2	J	149	VAL	2.0
1	M	156	PRO	2.0
1	M	183	SER	2.0
2	J	190	VAL	2.0
2	J	184	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.